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A new three-parameter cloud/aerosol particle size distribution based on the generalized inverse Gaussian density function

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Abstract

We describe a three-parameter cloud/aerosol size distribution based on the generalized inverse Gaussian density function that provides a simple and convenient recipe for characterizing aerosol radiative properties. The feature that makes this distribution attractive is that all of its moments can be calculated analytically providing simple formulas for the effective radius and variance and relating these to other important quantities such as the particle number and mass densities. Another advantage of this distribution is the smooth exponential cut-off not only for large particles sizes but also in small particles regime which prevents the singularity that occurs at zero size for large effective variances for distributions like the popular gamma distribution. Unlike most size distributions in current use the proposed functional form has a third-parameter (order) which provides greater flexibility in representing different distributional shapes. Analytical expressions for the moments of the generalized inverse Gaussian distribution in the generic case contain ratios of modified Bessel functions, however for half-integer orders these expressions are simple ratios of polynomials. As a practical example we compare extinction efficiency factors and asymmetry parameters computed for several different orders of the proposed distribution function. © 2000 Published by Elsevier Science Inc. All rights reserved.

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1. Introduction

For radiative transfer purposes, the area weighted effective radius r_{eff} and effective variance v_{eff} provide a robust description of the size distribution of cloud or aerosol particles. This has been shown to hold true in radiative transfer modeling of reflected and transmitted light for a wide range of popular size distributions such as the gamma, power law, and log-normal distributions [1]. This however is not the case for other important quantities such as the particle number density and the concentration of cloud condensation nuclei (CCN), which may differ by orders of magnitude between the gamma and log-normal distributions having identical values of r_{eff} and v_{eff}, particularly when the effective variance is large. To address the problem quantitatively and to provide more options for relating the particle number and mass densities to the area weighted radiative parameters we propose to adopt the generalized inverse Gaussian distribution as a new cloud/aerosol particle size distribution.

The inverse Gaussian distribution is known to mathematical and physical communities since 1915 when it was used independently by Schrödinger and Smoluchovski in their works on Brownian motion. Comprehensive review of its statistical properties and applications along with historical notes and extensive bibliography can be found in [2]. Here we note only that the name "inverse Gaussian" comes from the observation that the cumulant function of this distribution is the inverse of the cumulant function of the normal law. Below we refer to this original distribution as the "standard" distribution.

The inverse Gaussian function was introduced to radiative transfer theory by Malkmus [3] in 1967 as an alternative to the statistical (Goody) model to describe more accurately the probability density distribution of absorption coefficient strengths for water vapor. Since then, partly because of its desirable analytic properties, this distribution has found wide use in radiative transfer modeling of non-gray gaseous absorption (see e.g., [4,5]).

The generalization of the inverse Gaussian distribution (by adding an extra parameter (order)) was proposed in 1953 by Good [6]. A thorough analysis of the statistical properties of this generalized distribution is presented in [7]. In the present study we propose adoption of the generalized inverse Gaussian density function as a useful and flexible model for cloud and aerosol particle size distributions. Using this distribution in Mie theory computations provides the standard representation of aerosol radiative parameters (such as extinction efficiency factor and asymmetry parameter) with an additional dependence on the distribution order.

Advantages of this type of distribution include simple analytical expressions for all of its moments, effective radius and variance, as well as smooth exponential cut-off not only for large particles sizes but also in small particle region. This prevents the singularity at zero size for large effective variances. (Such singularity is a characteristic of the gamma distribution.) The proposed distribution has a third-parameter (order) in addition to effective radius and variance which accommodates a variety of different functional shapes.

Below we give definitions of the generalized inverse Gaussian distribution and present explicit expressions for moments, effective radius and variance both in general and for some important specific cases. Following this we discuss the application of this distribution in Mie theory computations of the extinction efficiency factor and asymmetry parameter for typical aerosol particle size ranges.

2. General form

We define the generalized inverse Gaussian particle size distribution function by the formula

$$n_v(r) = \frac{1}{2K_{v+1}(1/w)} \frac{r^v}{s^{v+1}} \exp\left[-\frac{1}{2w}\left(\frac{s}{r} + \frac{r}{s}\right)\right], \tag{1}$$

where r is particle radius, K_μ the modified Bessel function of the third kind with index μ. The parameter w represents the width of the distribution, s is an effective size parameter, and v is the order of the distribution, which can be an arbitrary real number (e.g., the standard inverse Gaussian distribution used in the Malkmus model [3] has order $-3/2$). This distribution is normalized by the condition

$$\int_0^\infty n_v(r)\, \mathrm{d}r = 1, \tag{2}$$

and has maximum at

$$r_{\mathrm{mode}} = \left(vw + \sqrt{1 + v^2 w^2}\right) \cdot s. \tag{3}$$

The moments of the distribution (1) have simple analytical form

$$\langle r^m \rangle = \int_0^\infty r^m n_v(r)\, \mathrm{d}r = b_m s^m, \quad \text{where } b_m = b_m(w) = \frac{K_{m+1+v}(1/w)}{K_{1+v}(1/w)}. \tag{4}$$

The effective radius and variance [1] are defined as

$$r_{\mathrm{eff}} = \frac{\int_0^\infty r\pi r^2 n(r)\, \mathrm{d}r}{\int_0^\infty \pi r^2 n(r)\, \mathrm{d}r} = \frac{\langle r^3 \rangle}{\langle r^2 \rangle}, \tag{5a}$$

$$v_{\mathrm{eff}} = \frac{1}{r_{\mathrm{eff}}^2} \frac{\int_0^\infty (r - r_{\mathrm{eff}})^2 \pi r^2 n(r)\, \mathrm{d}r}{\int_0^\infty \pi r^2 n(r)\, \mathrm{d}r} = \frac{\langle r^4 \rangle \langle r^2 \rangle}{\langle r^3 \rangle^2} - 1, \tag{5b}$$

they have the following form for the generalized inverse Gaussian distribution (1):

$$r_{\mathrm{eff}} = \frac{b_3}{b_2} \cdot s = \frac{K_{4+v}(1/w)}{K_{3+v}(1/w)} s, \tag{6a}$$

$$v_{\mathrm{eff}} = \frac{b_4 b_2}{b_3^2} - 1 = \frac{K_{5+v}(1/w) K_{3+v}(1/w)}{K_{4+v}^2(1/w)} - 1. \tag{6b}$$

Knowledge of the effective radius and variance obtained for example by means of remote sensing together with the aerosol optical depth τ (at some reference wavelength λ) allows us to calculate such an important physical quantities as the aerosol column mass loading per unit area

$$M = \frac{4}{3} r_{\mathrm{eff}} \rho \frac{\tau(\lambda)}{Q_{\mathrm{ext}}(\lambda, r_{\mathrm{eff}}, v_{\mathrm{eff}})},$$

where ρ is the aerosol specific density and Q_{ext} is the extinction efficiency factor that can be computed in the framework of Mie theory given r_{eff} and v_{eff}. (Note, that the ratio τ/Q_{ext} is spectrally invariant.)

Asymptotic behavior of r_{eff} and v_{eff} as functions of s and w in the limits $w \to 0$ and $w \to \infty$ is determined by the properties of the modified Bessel function K_μ [8]

$$K_\mu(z) \sim \sqrt{\frac{\pi}{2z}}\, \mathrm{e}^{-z} \left(1 + \frac{4\mu^2 - 1}{8z} + \cdots \right), \quad z \to \infty, \tag{7a}$$

$$K_\mu(z) \sim \frac{1}{2} \Gamma(\mu) \left(\frac{z}{2}\right)^{-\mu}, \quad z \to 0, \; \mu > 0. \tag{7b}$$

It follows from (7a) that in the case of very narrow distribution ($w \to 0$) $r_{\mathrm{eff}} \to s$, $v_{\mathrm{eff}} \to 0$. In the limit of very wide distribution ($w \to \infty$) the asymptotic limits of r_{eff} and v_{eff} have simple expressions in the following cases:

$$r_{\mathrm{eff}} = 2(3+v)ws \quad \text{for } v > -3 \quad \text{and } r_{\mathrm{eff}} = -\frac{1}{2(4+v)} w^{-1} s \quad \text{for } v < -4, \tag{8}$$

$$v_{\mathrm{eff}} = \frac{1}{3+v} \quad \text{for } v > -3 \quad \text{and } v_{\mathrm{eff}} = -\frac{1}{5+v} \quad \text{for } v < -5. \tag{9}$$

The last formula shows the upper bound for v_{eff} as a function of v. Note that the effective variance is unbounded when $-5 < v < -3$. The asymptotic value of r_{eff} becomes a decreasing function of w when $v < -7/2$.

The restricted range of the effective variance clearly reduces the practical utility of the distributions with large positive and negative orders. Nevertheless, the range of v for which the maximal value of v_{eff} is reasonably large, is still quite wide: e.g., $\max(v_{\text{eff}}) > 0.2$ for all v between -9.5 and 1.5.

3. Half-integer orders

Expressions for the moments of the generalized inverse Gaussian distribution become substantially simpler when the order v is half-integer, i.e.,

$$v = n - \frac{1}{2}, \tag{10}$$

where n is an integer. In this case modified Bessel functions K_μ can be expressed in terms of elementary functions [8]

$$K_{m+1/2}(z) = \sqrt{\frac{\pi}{2z}}\,\mathrm{e}^{-z}\sum_{k=0}^{m}\frac{(m+k)!}{k!(m-k)!}(2z)^{-k}. \tag{11a}$$

This allows us to express the distribution function (1) as well as its moments and effective radius and variance in terms of certain polynomials $P_m(w)$

$$n_{n-1/2}(r) = \frac{1}{\sqrt{2\pi w}P_n(w)}\frac{r^{n-1/2}}{s^{n+1/2}}\,\exp\left[\frac{1}{2w}\left(2-\frac{s}{r}-\frac{r}{s}\right)\right], \tag{11b}$$

$$\langle r^m\rangle = b_m s^m, \quad \text{where } b_m = \frac{K_{m+n+1/2}(1/w)}{K_{n+1/2}(1/w)} = \frac{P_{m+n}(w)}{P_n(w)}, \tag{12}$$

$$r_{\text{eff}} = \frac{P_{n+3}(w)}{P_{n+2}(w)}\cdot s, \quad v_{\text{eff}} = \frac{P_{n+4}P_{n+2}}{P_{n+3}^2} - 1. \tag{13}$$

The polynomials $P_m(w)$ are defined by the following formulas:

$$P_m(w) = \sum_{k=0}^{m}\frac{(m+k)!}{2^k k!(m-k)!}w^k, \tag{14a}$$

when $m \geqslant 0$ and

$$P_m(w) = P_{-m-1}(w), \tag{14b}$$

when $m < 0$. (The last relation follows from the symmetry property of the modified Bessel functions: $K_v(z) = K_{-v}(z)$.) These polynomials obey the following recursive relations:

$$P_{m+1}(w) = (2m+1)wP_m(w) + P_{m-1}(w), \tag{15}$$

$$w^2P_m'(w) = (mw-1)P_m(w) + P_{m-1}. \tag{16}$$

The first several polynomials are

$$\begin{aligned}
P_0 &= 1, \\
P_1 &= 1 + w, \\
P_2 &= 1 + 3w + 3w^2, \\
P_3 &= 1 + 6w + 15w^2 + 15w^3, \\
P_4 &= 1 + 10w + 45w^2 + 105w^3 + 105w^4, \\
P_5 &= 1 + 15w + 105w^2 + 420w^3 + 945w^4 + 945w^5.
\end{aligned}$$

It follows from the remarks in Section 2, that the upper bound of v_{eff} is reasonably high (greater than 0.2) for the half-integer orders $v = n - 1/2$ over the range where $n = -9, -8, \ldots, 0, 1, 2$.

Fig. 1 displays plots of the generalized inverse Gaussian distributions of the order $-7/2$ with $r_{\mathrm{eff}} = 1$ and various effective variances. The plots in Fig. 2 show dependence of the distribution at hand on its order v when both effective radius and variance are fixed ($r_{\mathrm{eff}} = 1$, $v_{\mathrm{eff}} = 0.2$). It is seen that both the position and value of the distribution maximum decrease with order. Comparison between the generalized inverse Gaussian distributions (of orders $-3/2$ and $-7/2$) with the log-normal and gamma distributions are presented in Fig. 3 (again $r_{\mathrm{eff}} = 1$ and $v_{\mathrm{eff}} = 0.2$ for all distributions). The plots show that the

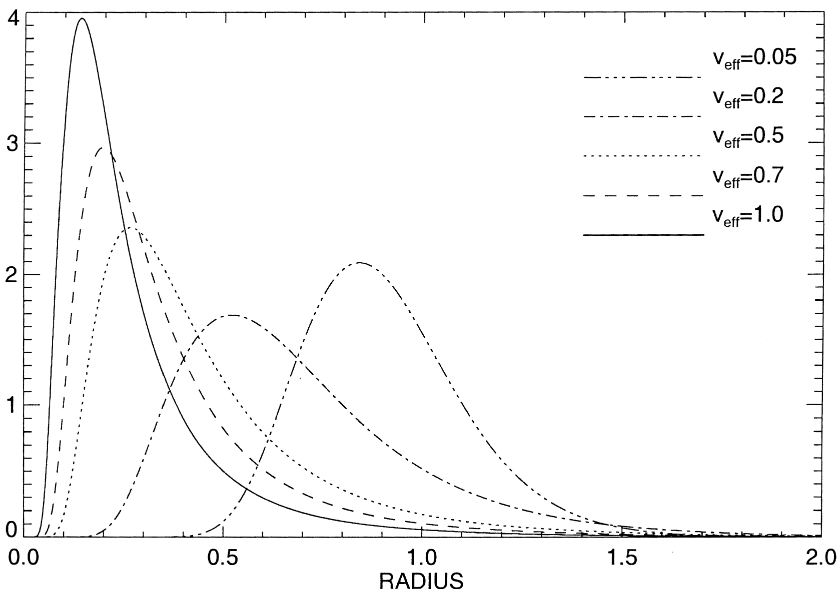


Fig. 1. The generalized inverse Gaussian distribution functions of the order $-7/2$ with $r_{\mathrm{eff}} = 1$ and various effective variances.

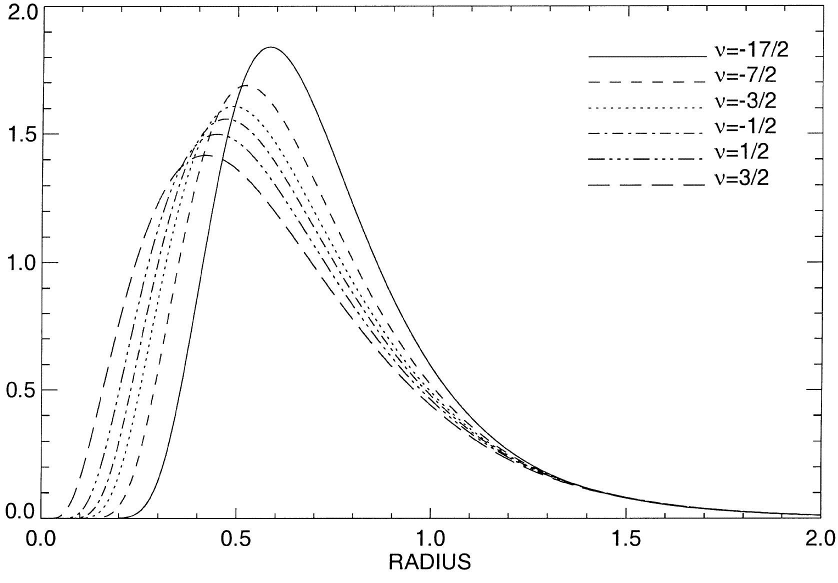


Fig. 2. Dependence of the generalized inverse Gaussian distribution on its order ν for all plots $r_{\mathrm{eff}} = 1$, $v_{\mathrm{eff}} = 0.2$.

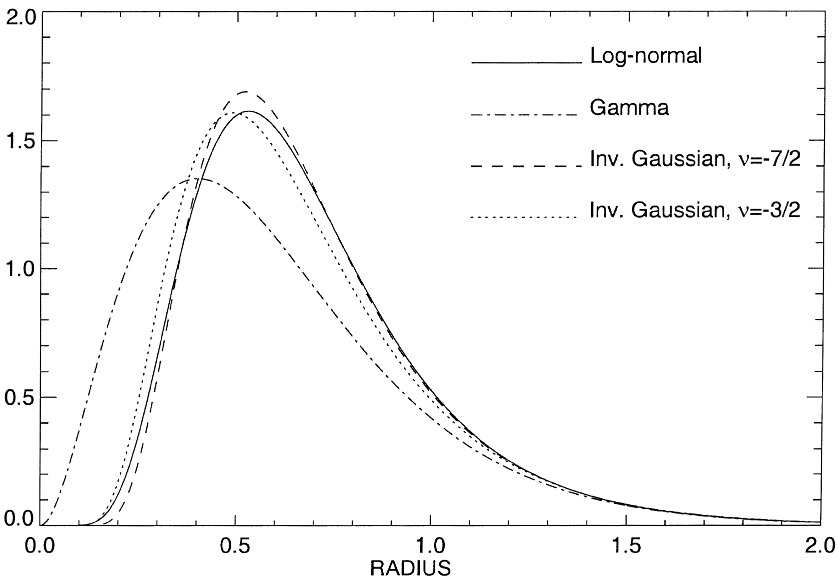


Fig. 3. Comparison between the generalized inverse Gaussian distributions (of orders $-3/2$ and $-7/2$) with the log-normal and gamma distributions ($r_{\mathrm{eff}} = 1$, $v_{\mathrm{eff}} = 0.2$ for all distributions).

log-normal and the generalized inverse Gaussian distribution of the order $-7/2$ are remarkably close approximations of each other especially when $r \sim r_{\mathrm{eff}}$.

4. Specific cases

Below we present explicit formulas for the generalized inverse Gaussian distribution of two specific orders. These are the standard (Malkmus model) distribution that is currently used to model gaseous absorption [2–4], and the special distribution ($v = -7/2$) which closely resembles the commonly used log-normal distribution.

4.1. Standard (Malkmus model) distribution ($v = -3/2$)

In this case $n = v + 1/2 = -1$ and $P_n = P_{-1} = P_0 = 1$. The distribution function and r_{eff} and v_{eff} have the following forms:

$$n_{-3/2}(r) = \frac{1}{\sqrt{2\pi w}} r^{-3/2} s^{1/2} \exp\left[\frac{1}{2w}\left(2 - \frac{s}{r} - \frac{r}{s}\right)\right], \tag{17}$$

$$\begin{aligned} r_{\mathrm{eff}} &= \frac{P_2}{P_1} s = \frac{1 + 3w + 3w^2}{1 + w} \cdot s, \\ v_{\mathrm{eff}} &= \frac{P_3 P_1}{P_2^2} - 1 = \frac{w(1 + 6w + 12w^2 + 6w^3)}{(1 + 3w + 3w^2)^2}. \end{aligned} \tag{18}$$

The effective variance in this case is bounded with the maximal value $2/3$, and $r_{\mathrm{eff}} = 3ws$ in the asymptotic value as $w \to \infty$.

The density distribution (17) also happens to be the inverse Laplace transform of the Malkmus band model transmission function [2,3]

$$T(u) = \exp\left[-\frac{\pi B}{2}\left(\sqrt{1 + \frac{4Su}{\pi B}} - 1\right)\right], \tag{19}$$

where $B = 2/(\pi w)$ is the effective line half-width and $S = s$ is the effective line strength, the physical parameters that apply when the distribution is used to represent gaseous absorption coefficient strength. This transmission function has provided a convenient formulation to model gaseous absorption in inhomogeneous media [3], particularly because of its useful feature that the density (17) can be integrated in closed form to yield the cumulative density distribution of absorption coefficient strengths including also the corresponding cumulative transmission function. This enables the transformation and subdivision of the absorption coefficient and transmission distributions into histogram form for convenient numerical computation without any loss of precision. We note here also that the Laplace transform of the density distribution (1) with an arbitrary v is a generalization of the transmission function (19). The generalized transmission function also has simple analytical form and desirable properties, however the details are not relevant to the present study.

4.2. Special distribution ($v = -7/2$)

We would like to single out this particular distribution because its effective radius and variance

$$r_{\mathrm{eff}} = \frac{P_0}{P_{-1}} \cdot s = s, \quad v_{\mathrm{eff}} = \frac{P_1 P_{-1}}{P_0^2} - 1 = P_1 - 1 = w \tag{20}$$

coincide precisely with the distribution defining parameters s and w. As a result this distribution is very convenient to use in that intermediate transformation of parameters is not necessary. (The gamma distribution has similar properties.) In this case $n = v + 1/2 = -3$ and $P_n = P_{-3} = P_2 = 1 + 3w + 3w^2$ and the distribution function (Fig. 1) has the following form:

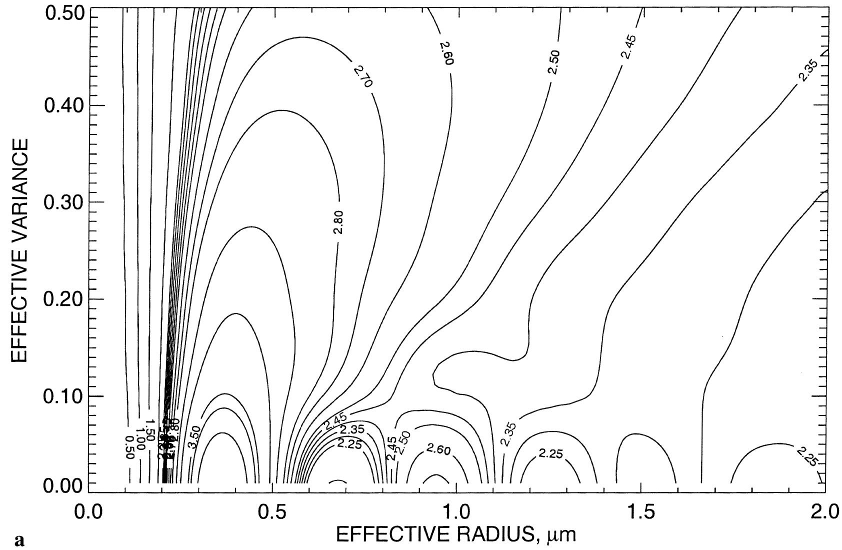
$$n_{-7/2}(r) = \frac{r^{-7/2} s^{5/2}}{\sqrt{2\pi w}(1 + 3w + 3w^2)} \exp\left[\frac{1}{2w}\left(2 - \frac{s}{r} - \frac{r}{s}\right)\right]. \tag{21}$$

As in the case of the log-normal distribution, the effective variance of the distribution at hand is unbounded. We have already noted, that there is an overall close resemblance of this distribution to the log-normal distribution for moderate values of radius (see Fig. 3). However, in the asymptotic regime ($r \rightarrow \infty$) the function (21) falls faster then the log-normal distribution function. This has the practical advantage of better convergence of integrals in numerical computations of radiative parameters.

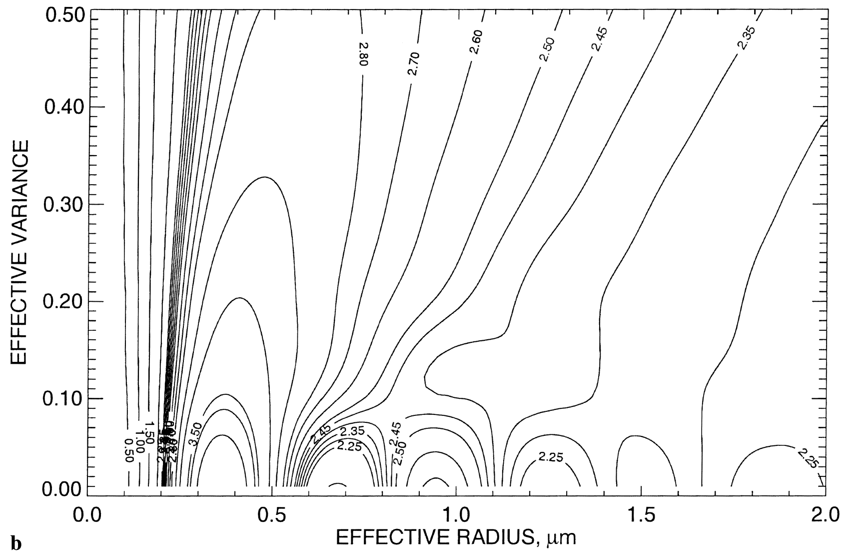
5. Computational results

Illustrative results of Mie theory for the extinction efficiency factor and asymmetry parameter [1] are obtained for the generalized inverse Gaussian particle size distributions of orders $-3/2$ and $-7/2$ and presented in Figs. 4 and 5. In both cases the calculations were performed at the reference wavelength of 550 nm for a representative aerosol refractive index with $n_r = 1.4$, $n_i = 0$ for full range of r_{eff} and v_{eff} that is also representative of atmospheric aerosols.

As expected, the contour plots in Fig. 4(a) and (b) (corresponding to $v = -3/2$ and $-7/2$, respectively) show great similarity of the extinction efficiency factor for small values of effective variance. This is because the radiative



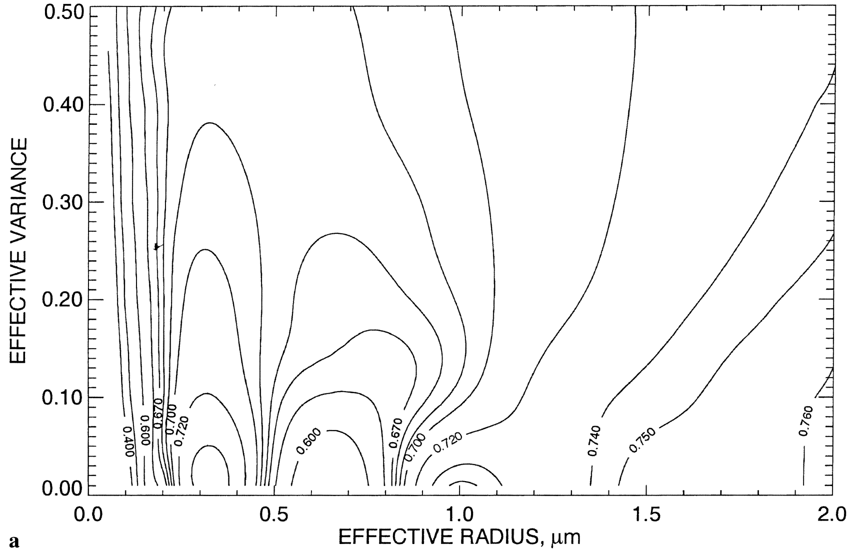
a



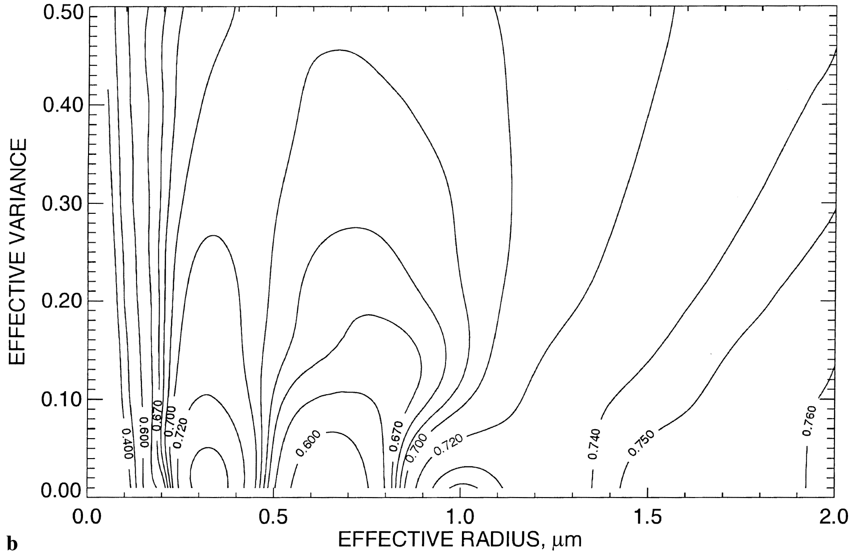
b

Fig. 4. (a)The extinction efficiency factor computed in the framework of the Mie theory (for 550 nm wavelength) using the generalized inverse Gaussian distribution of order $-3/2$; (b) The same as (a) but for the distribution of order $-7/2$.

parameters r_{eff} and v_{eff} (5a,b) were specifically defined to provide maximal independence of the results on the size distributions used [1]. Comparison between the two plots shows that larger differences occur only at relatively



a



b

Fig. 5. (a) The asymmetry parameter computed in the framework of the Mie theory (for 550 nm wavelength) using the generalized inverse Gaussian distribution of order $-3/2$; (b) The same as (a) but for the distribution of order $-7/2$.

large effective variances and for moderate values of $r_{\mathrm{eff}} \sim 0.5$ μm (which correspond approximately to the incident wavelength). Fig. 5(a) and (b) suggest similar conclusions the asymmetry parameter computations.

6. Discussion and conclusions

To be computationally useful, a size distribution must be both analytically simple and have desirable mathematical properties such as sharp exponential cut-offs in small and large particle regimes. The singularity of the gamma distribution at zero particle size for large values of effective variance and the slow convergence of the log-normal distribution in large particle size regimes are undesirable features of these commonly used distributions.

For most radiative transfer and remote sensing applications where particle size information is expressed in terms of r_{eff} and v_{eff}, the specific form of the size distribution rarely matters [1]. However, when there is a need to know the particle number density in terms of radiative parameters, there may be a great deal of uncertainty unless the form of the size distribution is known. For this purpose the proposed three-parameter generalized inverse Gaussian size distribution offers the advantage of flexibility that allows us to quantify the desired response of the computations to variations in the distribution functional shape.

We have demonstrated the generalized inverse Gaussian density function to be an analytically simple and flexible size distribution model. The obvious advantages of this distribution are analytic form of the expressions for all of its moments, effective radius and variance together with the smooth exponential cut-offs for both large and small particle sizes which keep the distribution non-singular even at large effective variances (see Fig. 1). Unlike most size distributions in current use in radiative calculations, the proposed functional form has a third-parameter (order) in addition to effective radius and variance which provides greater flexibility in fitting different distribution shapes (Fig. 2). For example, the distribution of the order $-7/2$ closely resembles the log-normal distribution at moderate radii while having better asymptotic behavior in the large particles regime. The effective variance of the generalized inverse Gaussian distribution may be bounded (like v_{eff} of the gamma distribution) or unbounded (like in the case of the log-normal distribution). The upper bound of the effective variance is reasonably large (greater then 0.2) for wide range of orders including the interval between -9.5 and 1.5.

Analytical expressions for the moments of the generalized inverse Gaussian distribution in the generic case contain ratios of modified Bessel functions, however for half-integer orders these expressions are simple ratios of polynomials. The class of such distributions includes the original inverse Gaussian distribution ($v = -3/2$) and the special distribution ($v = -7/2$) which effective radius and variance exactly coincide with the formal distribution parameters s and w that makes the use of this distribution very convenient.

As a practical example we compare extinction efficiency factors and asymmetry parameters computed for two different orders of the proposed distribution function. While showing the expected coincidence of the radiative parameters for small effective variances the results of the comparison also indicate some differences, especially for moderate r_{eff} and large v_{eff}. Such differences being relatively small still may be important in some remote sensing applications (especially in sensitivity studies), where using of the proposed size distribution can help to quantitatively estimate uncertainties of the retrievals due to a difference between the actual and model size distribution shapes.

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